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Optimal Cut of Langasite for High Performance SAW Devices

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Abstract. The results of a theoretical and experimental investigation of the SAW propagation characteristics in an optimal region of langasite defined by the Euler angles (–15°-+10°,120°-165°,20°-45°) are presented. Based on temperature coefficients of the elastic constants derived from experimental data, some optimal orientations of langasite characterized by high electromechanical coupling factor (k^2), zero power flow angle (PFA) and low or zero temperature coefficient of frequency (TCF) are found. It is shown that the SAW velocity in the region of interest is highly anisotropic, and this results in a significant amount of diffraction which must be taken into account in the search for orientations useful for SAW devices. An orientation having simultaneously zero PFA, zero TCF, negligible diffraction, and relatively high piezoelectric coupling has been found and verified experimentally. The experimental results are in excellent agreement with the calculated SAW characteristics. The frequency response of a SAW device fabricated on the optimal cut of langasite is presented and demonstrates that high performance SAW filters can be realized on this optimal cut of langasite.

I. Introduction

Recent progress in the development of communication systems has given rise to the further evolution of SAW devices which are often utilized as the key elements in such systems. The performance specifications required of these SAW devices can not always be realized if only the three customary crystalline materials are implemented as substrates: quartz, lithium niobate and lithium tantalate. Therefore, there is a strong need for new piezoelectric materials which can enhance the performance capabilities of SAW devices. First of all, to provide low insertion loss a new substrate material is expected to exhibit strong or moderately strong piezoelectric coupling. A new substrate must also provide minimal change of frequency with a corresponding change in temperature. At the same time SAW propagation on this new substrate must have minimal power flow angle and minimal diffraction. The substrate must also have a sufficiently high acoustic Q so that the SAW attenuation is acceptably low at high frequencies. It is not difficult to find substrates which provide any of these desireable properties, but it is not possible to satisfy all of these requirements in a single orientation of any of the three commonly used materials. The challenge is to find a new material which has an orientation or range of orientations which will simultaneously satisfy all of these requirements.

In addition to these technical requirements a new material needs to be commercially available at a reasonable price, which means that the growth technique can not be very complicated and expensive. It must be possible to grow large-size crystals with a diameter of at least 3 inches. For most commercial applications a low SAW velocity is preferred in order to minimize the chip and package size and consequently to reduce the cost of the SAW device.

At present only one piezoelectric material is definitely known to satisfy all these requirements. It is lanthanum gallium silicate $La_3Ga_5SiO_{14}$, or langasite. This crystal was synthesized in Russia in the early 1980-s [1] and soon proved to be a moderately strong piezoelectric with an electromechanical coupling factor a few times higher than that of quartz. Being isomorphous to quartz, (point symmetry class *32*) langasite "inherited" the specific temperature behavior of quartz including the existence of temperature compensated orientations for bulk and surface acoustic waves.

Langasite can be grown from melt by the well developed Czochralski method, and large size crystals of good quality have been successfully grown [2,3]. The propagation loss measured in langasite at GHz frequencies is lower than that in quartz [4] which makes langasite attractive for high-frequency devices. The absence of phase transitions up to the melting point T_0=1470°C opens the possibility of high-temperature applications. Compared to lithium niobate or lithium tantalate, langasite has an advantage of having a more stable chemical composition, due to a narrower region of homogeneity. Therefore, one can expect minimal variations in the SAW characteristics between as-grown crystals, though the same feature brings some difficulty into the growth process. One more advantage of langasite compared to customary SAW materials is the SAW velocity, which is lower than that of quartz by 15-30%.

The successful combination of these properties makes langasite a promising new material for future SAW devices provided that all these advantages are combined in at least one orientation. A numerical analysis of SAW characteristics in singly rotated cuts of langasite has revealed that none of these orientations exhibits simultaneously high piezoelectric coupling, low temperature coefficient of frequency (TCF) and small power flow angle (PFA). A thorough numerical investigation of SAW propagation characteristics in doubly rotated cuts has shown that there is a wide crystallographic area in which some optimal combinations of SAW properties can be obtained [5]. This area was defined by the following intervals of the Euler angle (φ,θ,ψ): $\varphi=-15°$-$+10°$, $\theta=120°$-$165°$, $\psi=20°$-$45°$. It includes the absolute maximum of electromechanical coupling factor k^2 for langasite (about 0.5%) and in a number of orientations moderately high coupling is combined with low or zero TCF and PFA values.

A conclusion that the mentioned area is distinguished by the excellent combination of SAW characteristics has been recently confirmed by several groups of researchers both theoretically and experimentally [6-8]. Experimental SAW characteristics have been reported for some promising orientations belonging to the optimal area, such as (0°,142°,24.5°) [6] or (0°,140°,22.5°) [8]. These and other orientations exhibit approximately equivalent combination of SAW characteristics with good temperature stability and moderately high piezoelectric coupling (k^2=0.3-0.4%).

Obviously, further theoretical and experimental work would be required in order to find the orientation with the best combination of these SAW properties. This paper presents the results of such work. The behavior of the main SAW characteristics is analyzed in the optimal area, including the anisotropy parameter (which determines the SAW diffraction effect and which was not taken into account by other researchers).

II. Investigation of SAW Propagation in the Optimal Area

A theoretical investigation of SAW characteristics must be based on reliable material data including the elastic, piezoelectric, and dielectric constants of the crystal and their temperature dependencies. A comparative analysis of published material constants of langasite [9-11] has shown that in general they give similar behavior of the SAW characteristics, except for the TCF. The electromechanical coupling factor is also sensitive to the choice of material data. For example, the absolute maximum of the coupling factor changes from k^2_{max}=0.46% to k^2_{max}=0.55% if the material constants from ref.[9] are replaced by the constants from ref.[10].

While selecting suitable material data for a theoretical investigation of the SAW behavior in the optimal area we focused on obtaining accurate values of PFA, anisotropy parameter, and TCF, the first two characteristics being dependent on the anisotropy of the SAW phase velocity. In Fig.1a the calculated and measured velocities are presented for SAW propagation in the Y+46.5° cut of langasite with Euler angles (0°, 136.5°, ψ). Calculations were based on three different sets of material constants [9-11]. In the structure used for the SAW measurements, the thickness of the aluminum electrodes was negligible (h/λ =0.002, where λ is the SAW wavelength). Fig.1a demonstrates that at least within the angular range considered by these curves the best agreement between calculated and measured SAW velocities is achieved when the material constants from ref.[10] are used. This conclusion agrees with the results obtained by other researchers [6]. Therefore, further calculations of SAW characteristics in the optimal area are based on the material constants from ref.[10].

A comparison of the experimental and calculated temperature characteristics of SAW propagation in the Y+46.5° cut of langasite (Fig.1b) has revealed that none of the reported sets of temperature coefficients of the material constants [9-11] describes the temperature dependence of frequency adequately, though all sets predict the existence of orientations with zero TCF in the optimal area. Therefore, improved temperature coefficients of the elastic constants were derived from the experimental dependence of TCF(ψ) in the Y+46.5° cut. They are the following: $Tc_{11}=-53$ ppm/°C, $Tc_{12}=-85$ ppm/°C, $Tc_{13}=-100$ ppm/°C, $Tc_{14}=-310$ ppm/°C, $Tc_{33}=-94$ ppm/°C, $Tc_{44}=-55$ ppm/°C. Though accurate simulation of material constants requires measurement of TCF in at least three mutually orthogonal crystal planes, the temperature coefficients found from experimental data for one plane provided excellent agreement between theoretical and experiment temperature behavior of the SAW in the Y+46.5° cut (Fig 1b) and in a wide area around it.

Using the simulated temperature coefficients and other material constants from ref.[10], the SAW characteristics were calculated in orientations of langasite defined by the Euler angles (-10°-+5°,135°-150°,ψ). In addition to the phase velocity V on a free surface, power flow angle ϕ, electromechanical coupling factor k^2 and TCF, the anisotropy parameter $\gamma=\partial\phi/\partial\psi$ has been calculated. It was found that for $\varphi=0$ and $\theta=135°$-$140°$ the TCF values do

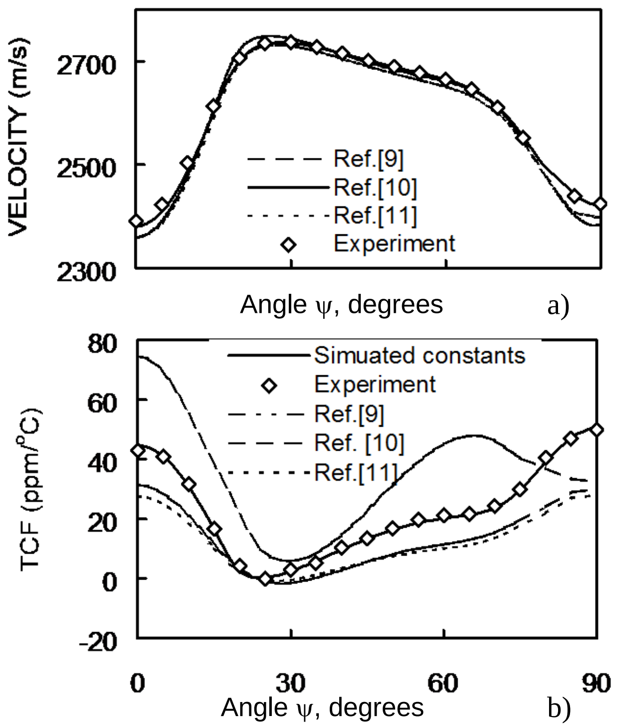

Fig.1. Calculated and experimental SAW velocities (a) and temperature coefficients of frequency(b) as functions of angle ψ in orientations of langasite with Euler angles (0°, 136.5°, ψ). The calculations are based on material constants from ref.[9-11] and simulated temperature coefficients of elastic constants.

not exceed 4 ppm/°C if ψ=24°-30°. The PFA(ψ) dependence crosses the zero line for any θ and ψ in the area analyzed. The electromechanical coupling factor is maximum (k^2=0.55%) in the orientation (–10°,145°, 12°).

However, the orientations with high coupling must be implemented with care because of the strong anisotropy in the propagation velocity. Even a small misalignment of 1° from the desired crystal orientation can result in dramatic beam steering, up to 10°. Also a strong diffraction effect is expected in these orientations which can cause degradation of the device performance and an increase in the insertion loss. The anisotropy parameter is extremely high around the orientation (0°,150°,22.5°) in which $|1+\gamma| \approx 12$. Besides, in this orientation the SAW velocity is very close to that of the shear bulk wave and coupling of the SAW with a parasitic bulk wave can occur. On the other hand, due to the strong anisotropy in the region of interest some cuts with γ=–1 can be found in which full autocollimation of the acoustic beam is expected. For example in orientations with Euler angles (0°,135°-140°,26°-27°), in addition to a small PFA (<3°) and low TCF (<2 ppm/°C) nearly zero diffraction can be predicted.

Calculated SAW characteristics for some orientations with zero PFA and various electromechanical coupling factors are presented in Table I. The main drawback of using langasite orientations with coupling factors k^2=0.47-0.54% is strong diffraction. On the other hand, in orientations with low diffraction the coupling factors are not so high. Thus the calculations show that the choice of a specific orientation in the optimal area depends on the relative priorities placed upon the various SAW propagation characteristics that we desire to optimize.

Table 1
SAW characteristics in some orientations of LGS with zero power flow angle

Euler angles	V (m/s)	k^2 (%)	TCF (ppm/°C)	γ
(0°,150°,24°)	2765	0.51	7	–4.9
(5°,150°,29°)	2798	0.50	3	–5.5
10°,150°,34°)	2829	0.47	–1	–5.9
(5°,145°,29°)	2793	0.42	–2	–2.3
(0°,140°,25.5°)	2747	0.37	1	–1.2
(0°,138.5°,26.3°)	2743	0.34	1	–1.0

III. AN OPTIMAL CUT OF LANGASITE WITH ZERO PFA, ZERO TCF AND ZERO DIFFRACTION

If none of the three Euler angles is fixed, it is possible to find an orientation in 3-dimensional space (φ,θ,ψ) in which the SAW is characterized simultaneously by TCF=0, PFA=0 and γ= –1. Indeed, each of these SAW properties becomes optimal if the corresponding orientation belongs to the characteristic surface in 3D space. Any characteristic surface, for example one defined by PFA=0, can be described in coordinates (φ,θ,ψ) as φ(θ,ψ). Two requirements, for example PFA=0 and γ= –1, can be satisfied simultaneously with a curve in 3D space which can be found as the intersection of the corresponding characteristic surfaces. Obviously, there can exist a point where this line intersects the third characteristic surface, TCF=0. In Fig.2a the line of orientations (φ,θ,ψ) characterized by PFA=0 and γ= –1 is presented by its projections θ(φ) and ψ(φ) onto the coordinate planes. The corresponding SAW velocity, k^2 and TCF are illustrated in Fig.2b,c as functions of φ. The temperature behavior of the SAW has been analyzed for

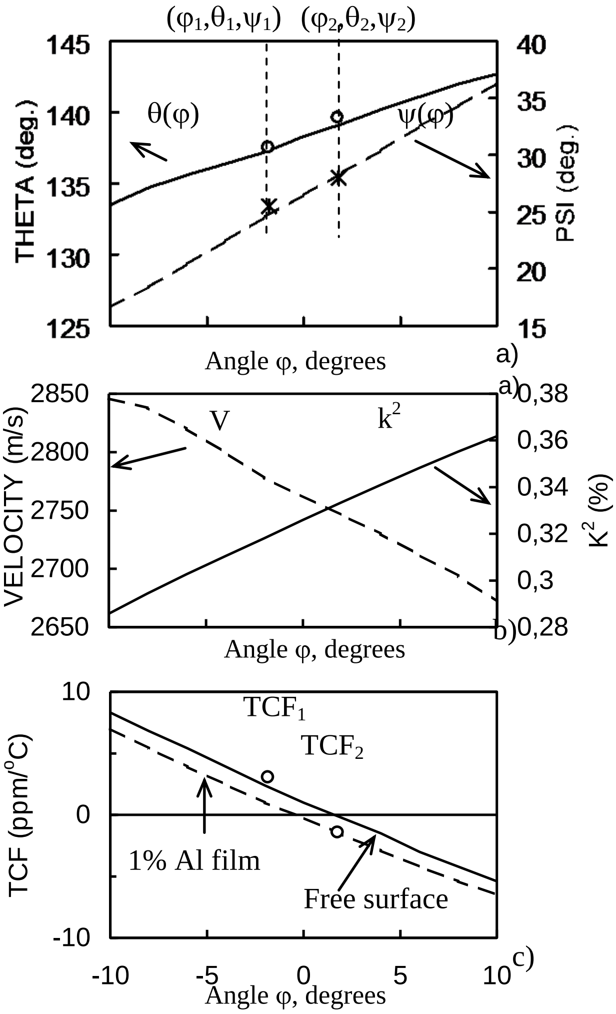

Fig.2. Calculated orientations of langasite (φ,θ,ψ) characterized by PFA=0 and $\gamma=-1$, plotted as $\theta(\varphi)$ and $\psi(\varphi)$ (a), SAW velocity, k^2 (b) and TCF (c) in these orientations. Two cuts with PFA=0 and $\gamma=-1$, ($\varphi_1,\theta_1,\psi_1$) and ($\varphi_2,\theta_2,\psi_2$), were experimentally verified.

two cases: when the surface is free and when it is covered by an aluminum overlay with a thickness $h/\lambda=0.01$. On the free surface TCF=0 occurs in the orientation (1.8°, 139°, 28°) while on the metallized surface with $h/\lambda=0.01$ the calculated optimal cut characterized by PFA=0, $\gamma=-1$ and TCF=0 is defined by the Euler angles (-0.5°, 138°, 26.5°).

To verify these calculations, an experimental investigation of the SAW propagation characteristics has been performed in orientations described by $\varphi=-4°$ - +2°, θ=134°-139° and ψ=20°-30°. As a result, two orientations have been found in which PFA=0 and $\gamma=-1$ occur simultaneously. In Fig.2a these orientations, ($\varphi_1,\theta_1,\psi_1$)

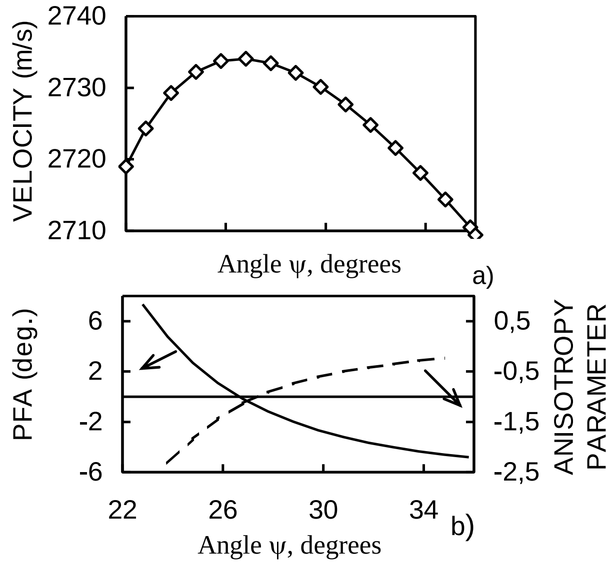

Fig3. Experimental SAW velocity (a), PFA and anisotropy parameter (b) as functions of angle ψ in orientations with Euler angles (0°, 138.5°, ψ).

and ($\varphi_2,\theta_2,\psi_2$), are presented as $\theta_1(\varphi_1),\psi(\varphi_1)$ and $\theta_2(\varphi_2),\psi_2(\varphi_2)$, respectively. The corresponding points nearly lie on the calculated lines which proves that there is good agreement between the numerical and experimental results and enables one to predict with high accuracy the optimal cut combining PFA=0, $\gamma=-1$ and TCF=0. Taking into account the experimental TCF values in these two orientations (Fig.2b) the optimal cut is (0.5°, 139°, 27°) when the aluminum thickness is negligible. With a very minor compromise in performance the first Euler angle can be set to zero. This simplifies the cutting of wafers as well as reduces the potential for errors in wafer production. If $\varphi=0$, the optimal combination of properties PFA=0, $\gamma=-1$, TCF<1 ppm/°C is expected for SAW propagation in the orientation (0°, 138.5°, 26.8°).

In Fig.3a the measured SAW velocities are plotted versus propagation angle ψ in the Y+48.5° rotated cut of langasite with Euler angles (0°, 138.5°, ψ) while Fig.3b illustrates the power flow angle and anisotropy parameter calculated from the measured velocities V(ψ). Zero PFA has been obtained at the point ψ=26.8° with V=2734 m/s, $\gamma=-1.17$, TCF≈0.

Zero temperature coefficient of frequency was achieved slightly above room temperature. Measured frequency-temperature characteristics for three propagation angles ψ =24.8, 26.8 and 28.8° near the optimal cut are

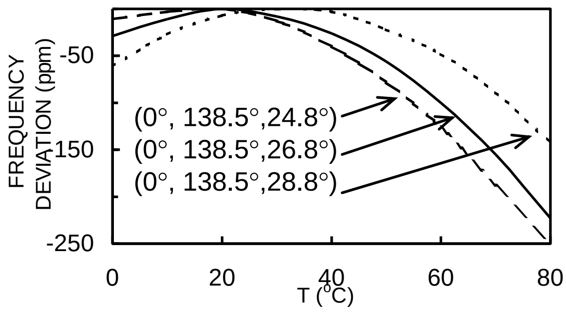

Fig.4. Frequency deviation versus temperature dependencies measured in three propagation directions on Y+48.5 cut of langasite, Euler angles (0°, 138.5°, ψ).

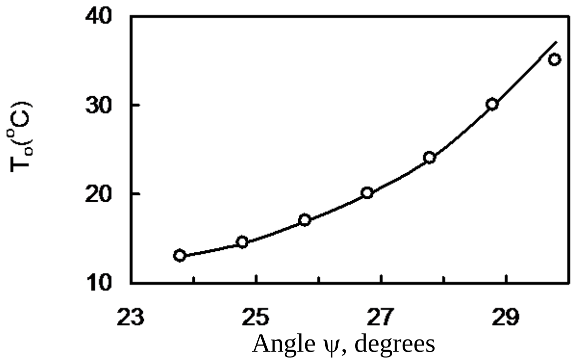

Fig.5. Measured turnover temperature as a function of angle ψ in orientations with Euler angles (0°, 138.5°, ψ).

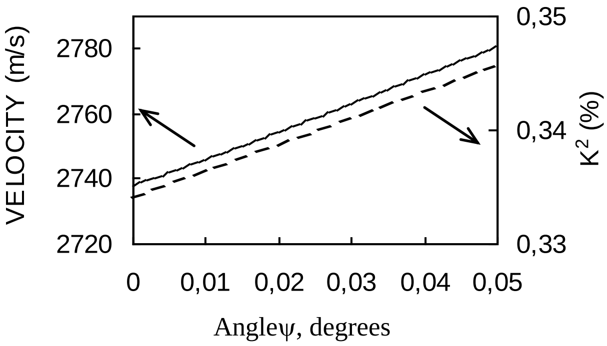

Fig.6. Calculated SAW velocity and electromechanical coupling factor as functions of normalized thickness of aluminum overlay in (0°,138.5°,26.8°) cut of langasite.

presented in Fig.4, and the experimentally determined turnover temperature T_0 is shown as a of angle ψ in Fig.5. In the interval 26.8±3° the turnover temperature varies between 10°C and 40°C.

Since the SAW velocity is higher in aluminum than in langasite, an aluminum overlay is expected to accelerate surface waves in this material. The calculated effect of a homogeneous aluminum film on the SAW velocity and electromechanical coupling factor is shown in Fig.6. Calculations have confirmed the increase in SAW velocity with metal thickness. The coupling factor is expected to grow and the turnover temperature moves to lower values with increasing Al thickness.

A typical frequency response of a bandpass filter device made on the optimal cut of langasite (0°, 138.5°, 26.6°) is presented in Fig.7. The bandwidth is 5.0 MHz centered at 200 MHz. The matched insertion loss is 16 dB, and the rejection is about 65 dB. The filter is implemented using tapered SPUDT electrode structures suitable for natural SPUDT substrates. The insertion loss could be decreased considerably since it is now dominated by resistive losses in the transducer electrodes. Since the transition bandwidth drops smoothly down to –68 dB, it can be concluded that there is no problem with diffraction, which is as one would expect when γ=–1.

IV. CONCLUSIONS

Theoretical and experimental investigations of the SAW propagation characteristics have been performed on orientations of langasite in a range defined by the Euler angles (–15°-+10°,120°-165°,20°-45°). Combining the elastic, piezoelectric and dielectric constants of Ilyaev et al. with temperature coefficients derived from experimental data provided excellent agreement between calculated and measured SAW characteristics. Orientations of langasite with zero PFA, small TCF, and various values of electromechanical coupling factors k^2 ranging from 0.34 to 0.51% have been found. Analysis of the anisotropy parameter has revealed that in orientations with higher coupling factors stronger SAW diffraction is expected. Orientations in which the SAW is characterized by zero power flow angle and full autocollimation (minimal diffraction) of the acoustic beam (γ=-1) have been calculated and presented as a line in a 3D space of Euler angles, and the accuracy of these results has been proved experimentally. Among these orientations the cut with TCF=0 has been discovered. For a negligible metal overlayer this cut is defined by the Euler angles (1.8°, 139°, 28°). Measured SAW data which involve a thin aluminum film indicates that the optimal defined by the angles (0°, 138.5°, 26.8°) where V=2734 m/s, PFA=0, γ= -1.17, TCF≈0. The frequency response of a SAW filter made on this orientation of langasite is presented.

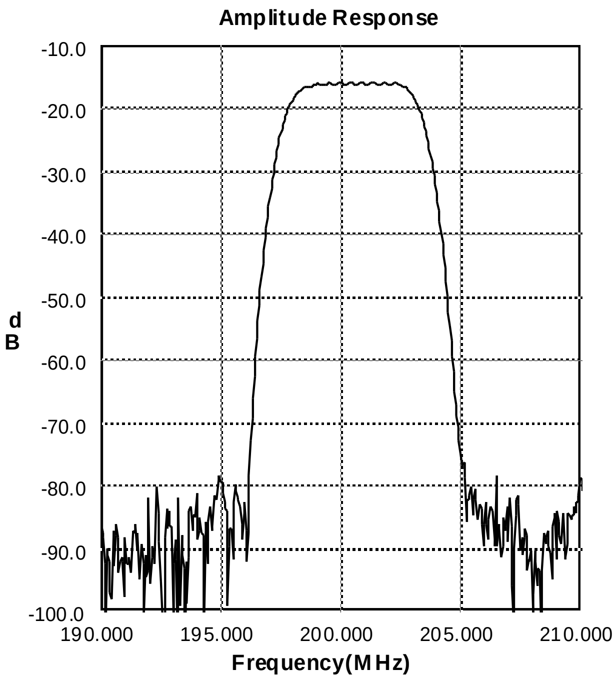

Fig.9. Frequency response of SAW filter with tapered SPUDT electrode structures, made on the optimal cut of langasite (0°,138.5°,26.6°).

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